Theory of field induced spin reorientation transition in thin Heisenberg films

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We consider the spin reorientation transition in a ferromagnetic Heisenberg monolayer with a second order single ion anisotropy as a function of temperature and external field. Up to now analytical methods give satisfying results only for the special case that the external field is aligned parallel to the easy axis of the crystal. We propose a theory based on a generalization of the Callen decoupling, which can be used for arbitrary direction of the external field. Excellent agreement between our results and Quantum Monte Carlo data is found for the field induced reorientation at finite temperatures. Additionally, we discuss the temperature dependence of the transition in detail.

I. INTRODUCTION

Since the discovery of the Giant Magneto Resistance (GMR) effect 1989[1] there has been enormous interest and research activity in the field of thin magnetic films. The magnetic anisotropy, merely a small perturbation in a bulk ferromagnet, gets strikingly important in thin film systems. Here the anisotropy is not only a necessary precondition of spontaneous ferromagnetism[2], but it determines many system properties as, e.g., the dependence of the magnetization vector or of the spin wave excitation spectrum on an applied magnetic field. Additionally, the anisotropy energy is of the same order of magnitude as the Interlayer Exchange Coupling (IEC)[3], which is intimately connected with the GMR effect. Thus an investigation of these effects has to take the magnetic anisotropy carefully into account.

There is an important phenomenon in thin ferromagnetic films which is closely connected to the magnetic anisotropy: the magnetic reorientation transition. This term denotes a rotation of the magnetization from the film normal into the plane or vice versa as a function of temperature, film thickness, or external magnetic field. The transition can be understood as a result of competing forces that favor different directions of the magnetization as e.g. spin orbit coupling, dipolar interaction, and an external magnetic field[4]. It can be described using a Heisenberg model in film geometry, with the usual Heisenberg exchange interaction, an external field, and one or more anisotropy terms.

For the simplest of these models,

$$H_1 = -\sum_{ij} J_{ij}\mathbf{S}_i\mathbf{S}_j - \sum_i \mathbf{B}_0\mathbf{S}_i, \tag{1}$$

consisting only of the exchange term and an external field, there are very accurate approximation schemes available. It was shown e.g. in Ref. 5 by comparison with QMC calculations, that the RPA decoupling[7] yields even quantitative results for the magnetization as a function of temperature.

Turning to anisotropy contributions, the spin-orbit coupling induced anisotropy is usually modelled by a single ion anisotropy

$$H_2 = -K_2 \sum_i S_{iz}S_{iz}, \tag{2}$$

which is of second order for systems with tetragonal symmetry. For film systems the z-axis is perpendicular to the film plane. If K_2 is positive the easy axis of the magnetization is the z-axis, for negative K_2 this is a hard direction. The RPA fails badly if applied to a local term as described in Eq. (2). Thus RPA can not be used to solve the whole model

$$H = H_1 + H_2. \tag{3}$$

In Ref. 8 an approximation for this model is proposed, which is based on a combination of the RPA approximation for the nonlocal terms (1) and an Anderson-Callen (A.C.) decoupling[10] for the local anisotropy contribution (2). This theory gives good results[6] for the magnetization if the anisotropy constant K_2 is much smaller than the exchange coupling J ($K_2 \leq 0.01J$) and if the external field is applied parallel to the z-axis while K_2 has to be positive. The first condition is not a serious restriction, since in reality the anisotropy constants are indeed much smaller than the Heisenberg exchange interaction. Furthermore this restriction can be relieved by an alternative theory[11]. The important restriction is given by the second condition. The described limit is a very special one, where both, the anisotropy as well as the external field favor a alignment of the magnetization parallel to the z-axis. Thus there are no "competing forces", and no magnetic reorientation transition occurs in this limit, which we want to refer to as "parallel limit" in the following. However, if the external field is not applied parallel to the z-axis and the magnetization is consequently rotated out of z, the approximation described in Ref. 8 looses its accuracy and becomes unacceptable for a quantitative description of the reorientation transition. This was shown in Ref. 6 by comparison with QMC calculations. Actually, to our knowledge there is no reliable model theory available, which can treat the model (3) for arbitrary directions of the external field or a negative anisotropy constant K_2.

However, such a model theory is highly desirable. It can be used to investigate quantitatively the magnetic reorientation transition in all systems dominated by second order lattice anisotropies. Numerical methods, as QMC calculations, are only applicable for the monolayer,

but a finite number of layers is crucial to study the interplay between surface and bulk anisotropies (see e.g. Ref. 4).
A priori, it is not clear, that such a model theory exists. The full model (3) is much more complex then the "parallel limit" case. The reason is that in that special case the total spin is a conserved quantity i.e. the total magnetization $\sum_i S_i^z$ commutes with the Hamiltonian. This property simplifies the calculations considerably but it is not present in the general model (3).
In this paper we want to show that nevertheless a well funded model theory can be formulated and that it is as accurate in the general case as in the "parallel limit". Comparing our results with the QMC data of reference[6] we will find excellent quantitative agreement for the magnetization and its components, which allows for a high quality description of the magnetic reorientation transition. The theory proposed in Ref. 8 is recovered for the special case of the "parallel limit".
In this paper we want to introduce the new theory and evaluate it by comparison with available QMC results. Since the latter are results for the monolayer, we will exclusively treat the case of a monolayer during this paper. A generalization to a multilayer system is straightforward.

II. THEORY

We will assume tetragonal symmetry in the following. The xy-plane is the film plane and thus the $x-$ and the $y-$ direction are equivalent. That is why we can confine the external field and the magnetization to the zx-plane without loss of generality. We will assume nearest neighbor coupling ($J_{ij} = J$ for nearest neighbors and $J = 0$ elsewhere) and for the explicit calculations a quadratic lattice. Let us first outline the main points of our theory. The aim is to calculate the angle and the norm of the total magnetization of the model (3).

1. In general, the magnetization is not aligned parallel to the z-axis. We therefore apply a coordinate transformation that rotates our system to align its z-axis parallel to the magnetization. The calculations are much easier and also more convenient in the new system referred to as Σ'.

2. After this we write down the equation of motion of the single magnon Green function. To solve this equation it is necessary to

3. decouple higher operator combinations. This appears to be straightforward for the exchange term (1) as long as one works in the rotated system Σ'. We will perform the usual RPA decoupling[7] here.

4. The situation is more complex for the anisotropy term (2). Here we will develop a new decoupling scheme following the ideas of the Callen decoupling[9]. However the original Callen decoupling is not applicable, since the total spin is not a conserved quantity in our model. Therefore the decoupling has to be generalized.

5. There is a special rotation angle $\hat{\theta}$ in our model: If the coordinate system is rotated by this angle $\Sigma \rightarrow \hat{\Sigma}$ and the decoupling procedure is applied, the total magnetization $\sum_i S_{i\hat{z}}$ commutes with the Hamiltonian (3). It is easy to show that $\hat{\theta}$ is therefore the direction of the magnetization. Now the condition $[\sum_i S_{i\hat{z}}, H]_- = 0$ gives an explicit expression for the magnetization angle.

6. Using the decouplings as well as the commutation property in the primed system we can solve the equation of motion and finally obtain the single magnon Green function as well as the norm of the magnetization $\langle S_{z'} \rangle$. Therewith the problem will be solved.

7. One can further show, that the effect of the anisotropy can be interpreted instructively as an effective "anisotropy field". We will calculate the components of this field.

Lets now follow this program in more detail. The rotation of the coordinate system is described by $\Sigma' = M\Sigma$, where M is a rotation matrix. Due to the symmetry we may confine the rotation to the zx-plane without loss of generality. This means that $y' = y$ and that the polar angle θ fully characterizes the rotation.

$$M = \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix}. \tag{4}$$

The z'-axis of the new system Σ' is set to be parallel to the magnetization direction. This gives:

$$\langle S_{x'} \rangle = \langle S_{y'} \rangle \; = \; 0. \tag{5}$$

The magnetizations in the fixed system Σ can now be read off from Eq. (4):

$$\begin{aligned} \langle S_x \rangle &= \sin\theta \langle S_{z'} \rangle, \\ \langle S_z \rangle &= \cos\theta \langle S_{z'} \rangle. \end{aligned} \tag{6}$$

$\langle S_z \rangle$ is the magnetization component normal to the film plane while $\langle S_x \rangle$ denotes the component parallel to the film plane. $\langle S_{z'} \rangle$, consequently, is the total magnetization. Of course, the angle θ is a priori unknown.

Next we want to write down the equation of motion of the single magnon Green function $G'_{ij}(E) = \langle\langle S_i^{+\prime}; S_j^{-\prime} \rangle\rangle$ defined in the new system. Applying the transformation (4) to the Hamiltonian (3) one readily finds:

$$EG'_{ij}(E) \; = \; \langle \left[S_i^{+\prime}, S_j^{-\prime} \right]_- \rangle + \langle\langle \left[S_i^{+\prime}, H \right]_- S_j^{-\prime} \rangle\rangle$$

$$
\begin{aligned}
&= 2\langle S_{z'}\rangle\delta_{ij} - 2J\sum_{l}^{\langle li\rangle}\left(\Gamma'_{ilj}(E) - \Gamma'_{lij}(E)\right)\\
&\quad +K_2(\cos^2\theta - \frac{1}{2}\sin^2\theta)\,\Gamma^{a'}_{ij}(E),\\
&\quad +(B_{x0}\sin\theta + B_{z0}\cos\theta)G'_{ij}(E)\\
&\quad -(B_{x0}\cos\theta - B_{z0}\sin\theta)\langle\langle S_i^{z'}; S_i^{-'}\rangle\rangle\\
&\quad +2K_2\cos\theta\sin\theta\langle\langle S_i^{z'}; S_i^{-'}\rangle\rangle\\
&\quad +2K_2\cos\theta\sin\theta\langle\langle {S_i^{z'}}^2; S_i^{-'}\rangle\rangle\\
&\quad -2K_2\cos\theta\sin\theta\langle\langle S_i^{+'}S_i^{x'}; S_i^{-'}\rangle\rangle
\end{aligned}
$$

with

$$
\begin{aligned}
\Gamma'_{mno} &= \langle\langle S_m^{z'}S_n^{+'}; S_o^{-'}\rangle\rangle \quad \text{and}\\
\Gamma^{a'}_{ij} &= \langle\langle S_i^{+'}S_i^{z'} + S_i^{z'}S_i^{+'}; S_j^{-'}\rangle\rangle. \qquad (7)
\end{aligned}
$$

The sum over l runs over the nearest neighbors of site i. The combination of trigonometric functions is a consequence of the rotation (4).

To proceed the operator products in Γ'_{mno} and $\Gamma^{a'}_{ij}$ have to be decoupled. For the nonlocal products in the former we choose a symmetric RPA decoupling $AB \to \langle A\rangle B + A\langle B\rangle$. Using Eq. (5) which is valid in the primed system we find

$$
S_m^{z'}S_n^{+'} \overset{RPA}{\longrightarrow} \langle S_{z\prime}\rangle S_n^{+'} \qquad (8)
$$

This is the same result as found in the original RPA approach[7] for the "parallel limit". Let us emphasize that this is only the case for the primed system Σ'. Thus the third point of our program is done.

The crucial fourth step introduces a new approximation scheme for the single ion anisotropy (2). It will be used to decouple the higher Green function $\Gamma^{a'}_{ij}$ as well as to treat operator combinations appearing in the commutator $[\sum_i S_{i\hat{z}}, H]_-$. The latter is important for the fifth step of our calculation.
1963 Callen introduced the Callen decoupling[9] which was intended as an improvement to the RPA decoupling[7]. The decoupling was performed at the Heisenberg exchange term (1). Later Anderson and Callen[10] used this proposal to treat the local anisotropy term (2) in the "parallel limit". Both approaches are based on the fact that the total magnetization commutes with the Hamiltonian, a condition that is not valid in our case. Therefore the procedure has to be rederived and generalized. We will not quite adopt the procedure as presented in Ref. 9 but rather use the main ideas.
The approximation makes use of the operator identity

$$
S(S+1) - S_x^2 - S_y^2 - S_z^2 = 0 \qquad (9)
$$

The spin operators work on the same site i, the site index is dropped here for convenience. Now the "zero" is added to the components of the spin operator, S_x, S_y, S_z:

$$
\begin{aligned}
S_{(x,y,z)} &= S_{(x,y,z)} +\\
&\quad \alpha_{(x,y,z)}\left(S(S+1) - S_x^2 - S_y^2 - S_z^2\right) \qquad (10)
\end{aligned}
$$

It is important to note that theses relations are identities for any $(\alpha_{(x,y,z)})$ only for exact calculations. On the contrary the result of some standard approximation procedure (e.g. of a symmetric mean field decoupling) changes if one uses the right hand side of Eq. (10) instead of the left hand side. The results do depend now on the prefactors $(\alpha_{(x,y,z)})$. It was the idea of Callen to use this degree of freedom to improve approximations. We will follow the proposal of Callen here and adjust the parameters in a way that interpolates between zero temperature and Curie temperature requirements. The explicit calculation is given in Appendix A. It gives:

$$
\alpha_{(x,y,z)} = \frac{\langle S_{(x,y,z)}\rangle}{2S^2} \qquad (11)
$$

Now we want to decouple operator combinations like $S_xS_z + S_zS_x$, $S_yS_z + S_zS_y$, or $S_xS_y + S_yS_x$ which appear in the equation of motion (7) in the higher Green function $\Gamma^{a'}_{ij}$. Thereto we replace the single operators by the right hand side of Eq. (10) and perform a symmetric decoupling procedure at the resulting expressions. Since the prefactors $\alpha_{(x,y,z)}$ are small quantities we neglect terms of the order α^2. For example the result for the operator combination $S_yS_z + S_zS_y$ is thus given by:

$$
\begin{aligned}
S_yS_z + S_zS_y \overset{A.C.}{\longrightarrow}\ & 2\langle S_y\rangle S_z + 2\langle S_z\rangle S_y \qquad (12)\\
& -2\frac{\langle S_y\rangle}{2S^2}\Big(\langle S_xS_z + S_zS_x\rangle S_x\\
& \quad +\langle S_yS_z + S_zS_y\rangle S_y + 2\langle S_z^2\rangle S_z\Big)\\
& -2\frac{\langle S_z\rangle}{2S^2}\Big(\langle S_xS_y + S_yS_x\rangle S_x\\
& \quad +2\langle S_y^2\rangle S_y + \langle S_zS_y + S_yS_z\rangle S_z\Big).
\end{aligned}
$$

For the other operator combinations analog expressions are found.
By virtue of relation (5) the result can be simplified if the decoupling is performed in the rotated coordinate system Σ'. We show in Appendix B that the following relations are fulfilled in Σ':

$$
\langle S_{a'}S_{b'} + S_{b'}S_{a'}\rangle = 0, \qquad (13)
$$

where a' and b' are two different subscripts out of (x', y', z'). This, together with Eq. (5), finally gives the decoupling within the parallel system Σ':

$$
\begin{aligned}
S_{x'}S_{z'} + S_{z'}S_{x'} &\overset{A.C.}{\longrightarrow} 0\\
S_{y'}S_{z'} + S_{z'}S_{y'} &\overset{A.C.}{\longrightarrow} 2\langle S_{z'}\rangle\left(1 - \frac{\langle S_{y'}^2\rangle}{S^2}\right)\cdot S_{y'}\\
S_{x'}S_{z'} + S_{z'}S_{x'} &\overset{A.C.}{\longrightarrow} 2\langle S_{z'}\rangle\left(1 - \frac{\langle S_{x'}^2\rangle}{S^2}\right)\cdot S_{x'} \qquad (14)
\end{aligned}
$$

Now the operator combination that appears in the Green function $\Gamma^{a\prime}_{ij}$ in the equation of motion (7) can be decoupled. Using Eq. (14) as well as the identity (9) one finds:

$$S_{+\prime}S_{z\prime} + S_{z\prime}S_{+\prime} \xrightarrow{A.C.} 2\langle S_{z\prime}\rangle C_1' S_{+\prime} \tag{15}$$

with

$$C_1' = 1 - \frac{1}{2S^2}\left(S(S+1) - \langle S_{z\prime}^2\rangle\right). \tag{16}$$

Using the decoupling procedures discussed up to now the higher Green functions Γ'_{mno} and $\Gamma^{a\prime}_{ij}$ in the equation of motion (7) can be treated. To treat the other four terms we have to address the fifth point of our program. Hence we will show in the following that for a certain angle $\hat{\theta}$ the total magnetization $\sum_i S_i^{z'}$ commutes with the Hamiltonian (3). Furthermore an explicit expression for the magnetization angle will be obtained.
Applying the rotation (4) to the Hamiltonian (3) and using the abbreviation $\gamma_1 = \sin\theta$ and $\gamma_2 = \cos\theta$ we find:

$$\begin{aligned}\left[\sum_i S_i^{z'}, H\right]_- &= \sum_i (\gamma_1 B_{z0} - \gamma_2 B_{x0})\cdot i S_i^{y'} \\ &\quad + K_2\gamma_1\gamma_2 \cdot i\left(S_i^{y'}S_i^{z'} + S_i^{z'}S_i^{y'}\right)\end{aligned}$$

Now the last operator product is decoupled according to Eq. (14). This gives:

$$\begin{aligned}\left[\sum_i S_i^{z'}, H\right]_- &= \sum_i \Bigg(\gamma_1 B_{z0} - \gamma_2 B_{x0} \\ &\quad + 2K_2\gamma_1\gamma_2\langle S_{z\prime}\rangle\Big(1 - \frac{\langle S_{y\prime}^2\rangle}{S^2}\Big)\Bigg)\cdot i S_i^{y'}\end{aligned} \tag{17}$$

Thus, in the framework of our approximation, the total magnetization indeed commutes with the Hamiltonian if the term in brackets on the right hand side is zero. This has important consequences: All expectation values and Green functions in the rotated coordinate system $\hat{\Sigma}$ that do not conserve the spin are zero in the framework of our theory. This can be seen using, e.g., the Lehmann representation of the Green function. In particular this applies for $\langle S_{+\prime}\rangle$ and $\langle S_{-\prime}\rangle$. Therefore Eq. (5) holds in this coordinate system which is thus found to be equivalent to the system Σ': $\hat{\Sigma} = \Sigma'$. Hence from Eq. (18) follows simple condition for the magnetization angle θ:

$$\begin{aligned}0 \stackrel{!}{=}\ & \sin\theta B_{z0} - \cos\theta B_{x0} \\ & + 2K_2 \sin\theta\cos\theta\langle S_{z\prime}\rangle C_1'\end{aligned} \tag{18}$$

The expectation value $\langle S_y^2\rangle$ is already evaluated here using the property of spin conservation in the primed system. Eq. (18) is our first important result.

Having calculated the magnetization angle now the norm of the magnetization $\langle S_{z\prime}\rangle$ has to be derived. This turns out to be a straightforward task. Due to the property of spin conservation in the primed system the Green functions in the last four lines of the equation of motion (7) are identical to zero. The remaining higher Green functions Γ'_{mno} and $\Gamma^{a\prime}_{ij}$ can be decoupled by Eqs. (8) and (14). Thus the equation of motion (7) can be solved after Fourier transformation. We finally obtain the single magnon Green function $G'_{\mathbf{q}}(E)$,

$$\begin{aligned}G'_{\mathbf{q}}(E) &= \frac{2\langle S_{z\prime}\rangle}{E - E'_{\mathbf{q}}} \\ \text{with} & \\ E'_{\mathbf{q}} &= 2\langle S_{z\prime}\rangle J(p - \gamma_{\mathbf{q}}) + B \\ B &= B_{x0}\sin\theta + B_{z0}\cos\theta \\ &\quad + K_2\left(\cos^2\theta - \frac{1}{2}\sin^2\theta\right)2\langle S_{z\prime}\rangle C_1'.\end{aligned} \tag{19}$$

The term p denotes the coordination number, while $\gamma_{\mathbf{q}}$ is a structural factor due to the Fourier transformation of the Heisenberg exchange term. For the quadratic lattice chosen here it is given by:

$$\gamma_{\mathbf{q}} = 2\left(\cos aq_x + \cos aq_y\right),$$

where a is the lattice constant. The trigonometric functions in Eq. (19) are obviously a consequence of the rotation. Knowing the Green function $G'_{\mathbf{q}}(E)$ one can calculate the desired expectation values in the primed system, i.e. the total magnetization $\langle S_{z\prime}\rangle$ and $\langle S_{z\prime}^2\rangle$ by a standard text book procedure[12] finally ending up with a self consistent system of equations. Before discussing the results of our theory in more detail we want to offer an instructive interpretation of the work of the anisotropy in the framework of our approximation. This will be the last point of our theory section.

The abbreviation B in Eq. (19) has the same effect on the Green function as an external field aligned parallel to the magnetization. Combining the expression for B with the magnetization angle, we may write down the components of the effective field:

$$\begin{aligned}B_x &= B\sin\theta \\ &= B_{x0} - K_2\langle S_x\rangle\sin^2\theta C_1' \\ &= B_{x0} + B_{xa} \\ B_z &= B\cos\theta \\ &= B_{z0} + 2K_2\langle S_z\rangle(1 - \frac{1}{2}\sin^2\theta)C_1' \\ &= B_{z0} + B_{za}.\end{aligned} \tag{20}$$

Obviously, the effective field may be written as a sum of the external field and an "anisotropy field" $\mathbf{B}_a = (B_{xa}, 0, B_{za})$. The anisotropy acts exactly like this field as far as the magnetization and the magnon energies $E_{\mathbf{q}}$ are concerned.

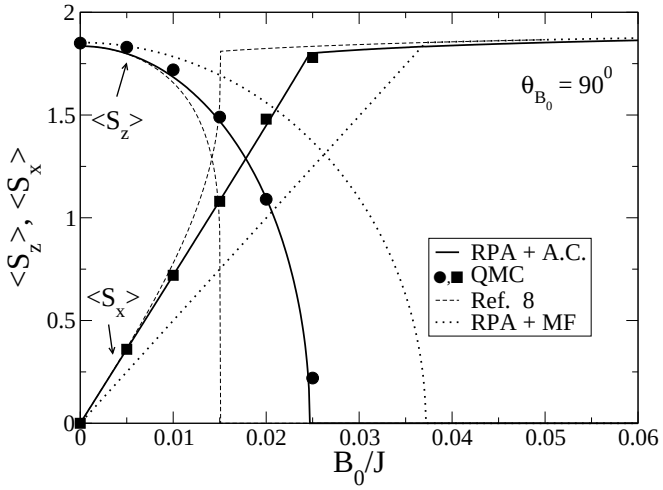

FIG. 1: The x- and the z-component of the magnetization $\langle S_x\rangle$, $\langle S_z\rangle$ as a function of the external field calculated with our RPA+A.C. approach (solid line), the approximation proposed in Ref. 8 (dashed line) and with a mean field decoupling of the anisotropy term (dotted line) in comparison with the QMC results from Ref. 6 (symbols). Parameters: $K_2 = +0.02J$ and $k_BT = 2J \approx 0.32k_BT_c, S = 2$.

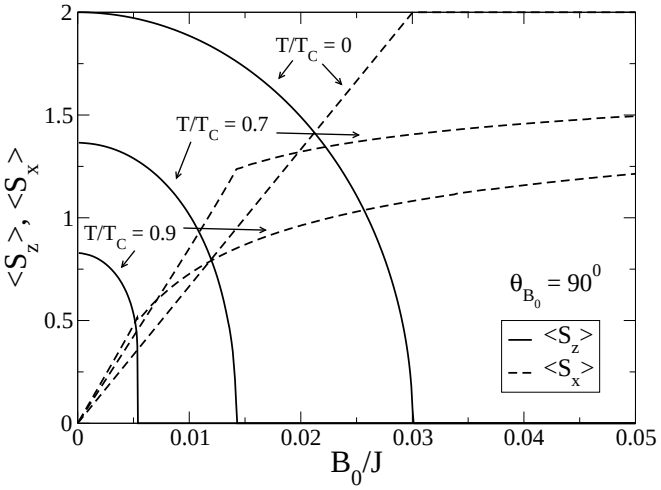

FIG. 2: The z-component $\langle S_z\rangle$ (solid lines) and the x-component $\langle S_x\rangle$ (dashed line) as a function of the external field B_{x0} applied within the film plane. Further parameters: $K_2 = 0.01J$, $S = 2$, k_BT_c equals $5.75J$.[13]

In the next section we will present the results of our theory and compare them with QMC data and other approximations.

III. RESULTS AND DISCUSSION

We start our discussion with a comparison of our results to QMC data of Ref. 6, which are free of systematic errors. Fig. 1 shows the results for the field induced reorientation transition at finite temperatures. A positive anisotropy constant ($K_2 > 0$) and an external field parallel to the film plane ($\theta_{B_0} = 90°$) are considered. The external field is applied perpendicular to the easy direction of the magnetization, a situation representing a severe test for our theory. The components of the magnetization $\langle S_x\rangle$ and $\langle S_z\rangle$ are shown as functions of the external field. For zero field the magnetization is aligned parallel to the easy axis. It is fully rotated into the film plane at the reorientation field B_{r0}. We display the results of our calculations (RPA+A.C. - solid lines) and the QMC results of Ref. 6 (symbols). Additionally the results of two other theories are shown for comparison: For the dotted line the anisotropy term (2) is treated by simple mean field decoupling:

$$S_i^z S_i^z \xrightarrow{MF} 2\langle S_z\rangle S_i^z \tag{21}$$

The dashed line shows the proposal of Ref. 8. Here the operator combination $S_i^+S_i^z + S_i^zS_i^+$ is decoupled as in the parallel limit treated in the original paper of Anderson and Callen[10]:

$$S_i^+S_i^z + S_i^zS_i^+ \to 2\langle S_z\rangle\left(1 - \frac{1}{2S^2}(S(S+1) - \langle S_z^2\rangle)\right). \tag{22}$$

The exchange term in all model calculations is treated by an RPA decoupling.

The results of our theory (solid lines) are in excellent agreement with the QMC data. We achieved even quantitative agreement for all magnetization angles θ. The quality of the approximation indeed turns out to be the same for all angles θ, which was the aim of this paper. Our approach is clearly superior to the approximation proposed in Ref. 8, to the mean field decoupling, and to all other approximations shown in Fig. 11 of Ref. 6. Fig. 1 visualizes our main result, namely that we succeeded to develop a theory for the extended Heisenberg model (3) that is as accurate as the RPA for the model (1). In the following we will discuss some additional features of the reorientation transition.

In Fig. 2 the temperature dependence of the transition is analyzed. Again, the components of the magnetization are displayed as a function of the external field, which is applied in the film plane, perpendicular to the easy direction. The calculations were performed for three different temperatures. Since the system is not saturated at finite temperatures, the total magnetization increases with the external field. This is seen best after the reorientation ($B_0 > B_{0r}$), where only one component of the magnetization ($\langle S_x\rangle$) is present. For higher temperatures the transition as a function of the external field becomes sharper. The reorientation field B_{0r} decreases faster with temperature than the zero field magnetization, reflecting the fact that the anisotropy becomes less important at higher temperatures. Another interesting feature is that the $x-$component increases linearly with

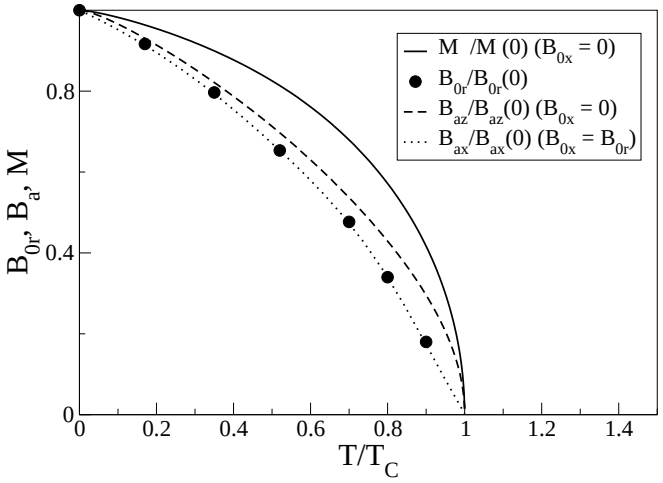

FIG. 3: The magnetization, the reorientation field B_{0r} (dots) and the anisotropy field B_a for $\theta = 0°$ (dashed line) and $\theta = 90°$ (dotted line) as a function of temperature. All quantities are scaled to their zero temperature value. The other parameters are as in Fig. 2. For Comparison scaled magnetization curves are added (solid line).

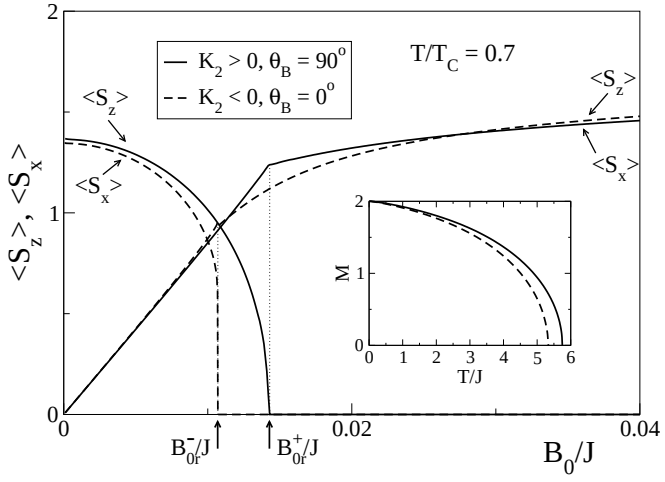

FIG. 4: The $z-$ and $x-$component of the magnetization as a function of the external field. Results for positive $K_2 = 0.01J$ (solid lines) and negative $K_2 = -0.01J$ (dashed lines) are shown, $T = 0.7T_c$. The small arrows highlight the position of the reorientation fields B_{0r}^+ for positive and B_{0r}^- for negative anisotropy. The inset shows the magnetization curves for $B_0 = 0$. The other parameters are as in Fig. 2.

the external field until the reorientation field is reached. This holds for all temperatures and is qualitatively different from the approximation proposed in Ref. 8. Qualitatively, this feature is also found in mean-field theory as can be seen in Fig. 1 of Ref. 14.

The observed behavior follows directly from Eq. (18). Since the external field is applied parallel to the film plane one finds for the x-component of the magnetization $\langle S_x \rangle$:

$$\begin{aligned} \langle S_x \rangle &= \sin\theta \, \langle S_{z'} \rangle \\ &= \frac{B_{x0}}{2K_2 C_1'(T)}. \end{aligned} \tag{23}$$

Since C_1' (Eq.19) increases with temperature, the slope of $\langle S_x \rangle$ is steeper for higher temperatures. Additionally, Eq. (23) determines the reorientation field B_{0r}. We find:

$$B_{0r}(T) = 2K_2 \langle S_{z'} \rangle(T) \, C_1'(T). \tag{24}$$

The fast decay of the reorientation field with temperature as compared to the magnetization is also due to the temperature dependence of C_1'.

This can also be seen in Fig. 3, where we considered the temperature dependence of the system in detail. We plotted the norm of the components of the anisotropy field (20) as well the reorientation field (circles) and the magnetization (solid line) as a function of temperature. All quantities are scaled to their zero temperature value. The anisotropy fields are plotted at their maxima, i.e. at $\theta = 0°$ for B_{az} (dashed line) and at $\theta = 90°$ for B_{ax} (dotted line). The temperature dependence of the anisotropy fields (20) as well as of the reorientation field (24) are determined by the factor $\langle S_{z'} \rangle(T) \, C_1'(T)$. Thus this quantities have nearly the same temperature dependence and their slopes are steeper than that of the magnetization $\langle S_{z'} \rangle(T)$ alone.

Very similar results are found for the easy plane case ($K_2 < 0$, $\mathbf{B}_0 \| z$). In Fig. 4 we compare both cases of a reorientation transition. Solid lines show the transition for an easy axis system, dashed lines denote the easy plane case. In the inset, the respective magnetization curves $M(T) = \langle S_{z'} \rangle(T)$ are plotted for zero external field. The Curie temperature and the magnetization at finite temperatures are somewhat smaller for the easy plane system. A reduced magnetization leads to a reduced reorientation field (see Eq. (24)). This explains the differences between both cases concerning the reorientation transition as seen in the main panel.

IV. CONCLUSIONS AND OUTLOOK

In this paper we addressed the magnetic reorientation transition in a Heisenberg monolayer as a function of the external field and temperature. The basis of our approach is a transformation of the Hamiltonian into a coordinate system Σ' (with the z' axis parallel to the magnetization) as well as a generalized Anderson-Callen decoupling procedure. Compared to the bare Heisenberg Hamiltonian (1), the problem is more complicated, since the total spin is not conserved. However, this complication turns out to be less serious, as it can be shown that the total spin is a conserved quantity in the framework of our approximation, if a appropriate quantization axis is chosen. This fact can be used to calculate the magnetization angle as well as to solve the equation of motion for the single magnon Green function. It was further shown that the effect of the

anisotropy can be described by an effective "anisotropy field".
Our results show a strikingly quantitative agreement with the QMC data of Ref. 6 yielding a significant improvement over all other decoupling schemes discussed so far (see e.g. Ref. 6). The main practical virtue of the new approach is that calculations can be performed as accurate as with QMC but much faster.
The theory can be generalized to a multilayer system and can thus be used for cases where QMC calculations are not feasible any more (e.g. thicker films). It should therefore be used to analyze the magnetic reorientation transition as a function of the film thickness as found in many transition metal films (see e.g. Ref. 4).
Due to its accuracy and convenience the theory shall further be used for a quantitative analysis of ferromagnetic resonance (FMR) experiments[15,16]. The decisive feature for the interpretation of a FMR experiment is the dependence of the $q = 0$ spin wave mode $E_{\mathbf{q}=0}$ on the external field $\mathbf{B}_0$. The function $E_{\mathbf{q}=0}(\mathbf{B}_0)$ can be easily calculated in our theory for any direction of the external field. This opens the possibility to extract the microscopic anisotropy constant K_2 directly from FMR experiments.

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Appendix A

In this Appendix we derive the prefactors of Eq. (10). We follow the philosophy of Callens paper[9] and calculate the prefactors as an interpolation between low and high temperatures. Lets start with the former limit $T \approx 0$:
Starting point is Eq. (10). We will consider expectation values instead of operators and transform the resulting expression as:

$$\begin{aligned}\langle S_z\rangle &= \langle S_z\rangle + \alpha_z\langle S(S+1) - S_x^2 - S_y^2 - S_z^2\rangle \\ &= \langle S_z\rangle + \alpha_z\langle S(S+1) - S_{x'}^2 - S_{y'}^2 - S_{z'}^2\rangle \\ &= \langle S_z\rangle \\ &\quad +\alpha_z\langle S(S+1) - S_{z'} - S_{-\prime}S_{+\prime} - S_{z'}^2\rangle \quad (25)\end{aligned}$$

The primed terms are quantities of the rotated system which is aligned parallel to the magnetization. Now the expectation values of the right hand side are approximated by their zero temperature values

$$\begin{aligned}\langle S_{z'}\rangle &\overset{T\to 0}{\longrightarrow} S \\ \langle S_{z'}^2\rangle &\overset{T\to 0}{\longrightarrow} S^2 \quad (26)\end{aligned}$$

This gives

$$\langle S_z\rangle \approx S\cos\theta + \alpha_z\langle -S_{-\prime}S_{+\prime}\rangle \quad (27)$$

If α_z is set to zero, the left hand side and the right hand side of Eq. (25) are approximated on the same level, i.e. the expectation values at low temperatures are replaced by their zero temperature value. However one can even improve the approximation for the left hand side by choosing α_z adequately. The choice

$$\alpha_z(T \approx 0) \overset{!}{=} \frac{\cos\theta}{2S} \quad (28)$$

recovers the free spin wave result

$$\langle S_z\rangle \approx \cos\theta\left(S - \frac{1}{2S}\langle S_{-\prime}S_{+\prime}\rangle\right) \quad (29)$$

On the other hand for high temperatures $T > T_c$ the left hand side of Eq. (25) has to vanish. This can be assured by the choice

$$\alpha_z(T > T_c) \overset{!}{\sim} \cos\theta\langle S_{z'}\rangle. \quad (30)$$

Combining the settings (28) and (30) one ends up with Eq. (11):

$$\alpha_z \overset{!}{=} \frac{\cos\theta\langle S_{z'}\rangle}{2S^2} = \frac{\langle S_z\rangle}{2S^2}. \quad (31)$$

Analog calculations lead to the prefactors α_x and α_y.

Appendix B

Here we want to derive the relation (13). Starting point is Eq. (5). First we want to calculate the expectation value $\langle S_{x'}S_{y'} + S_{y'}S_{x'}\rangle$. Using the decoupling (12) together with Eq. (5) one finds

$$\begin{aligned}\langle S_{x'}S_{y'} + S_{y'}S_{x'}\rangle &\rightarrow \langle S_{x'}\rangle\mathcal{A} + \langle S_{y'}\rangle\mathcal{B} \\ &= 0 \quad (32)\end{aligned}$$

The terms $\mathcal{A}$ and $\mathcal{B}$ are given by the decoupling procedure (12). This is one of three equations that have to be derived to prove relation (13). Next we want to treat $\langle S_{x'}S_{z'} + S_{z'}S_{x'}\rangle$. Using the decoupling rule (12) as well as the result (32) one finds:

$$\begin{aligned}S_{x'}S_{z'} + S_{z'}S_{x'} \rightarrow\ & 2\langle S_{z'}\rangle S_{x'} \\ & -2\frac{\langle S_{z'}\rangle}{2S^2}\Big(2\langle S_{x'}^2\rangle S_{x'} \\ & +\frac{1}{2}\langle S_{x'}S_{z'} + S_{z'}S_{x'}\rangle S_{z'}\Big)\end{aligned}$$

Thus it follows for the expectation value

$$\begin{aligned}\langle S_{x'}S_{z'} + S_{z'}S_{x'}\rangle \rightarrow\ & 2\langle S_{z'}\rangle\langle S_{x'}\rangle \\ & -2\frac{\langle S_{z'}\rangle}{2S^2}\Big(2\langle S_{x'}^2\rangle\langle S_{x'}\rangle \\ & +\frac{1}{2}\langle S_{x'}S_{z'} + S_{z'}S_{x'}\rangle\langle S_{z'}\rangle\Big)\end{aligned}$$

$$= -\frac{\langle S_{z'}\rangle}{2S^2}\left(\langle S_{x'}S_{z'} + S_{z'}S_{x'}\rangle\langle S_{z'}\rangle\right)$$

therefore:

$$0 = \langle S_{x'}S_{z'} + S_{z'}S_{x'}\rangle\left(1 + \frac{\langle S_{z'}\rangle^2}{2S^2}\right)$$

and

$$0 = \langle S_{x'}S_{z'} + S_{z'}S_{x'}\rangle \quad (33)$$

The equation

$$\langle S_{y'}S_{z'} + S_{z'}S_{y'}\rangle = 0 \quad (34)$$

is derived in a analog way. Eqs. (32), (33), and (34) prove relation (13).

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